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Decoherence and noise in spin-based solid state quantum computers. Approximation-free numerical simulations

ABSTRACT

This project has developed and used advanced high-precision numerical techniques to accurately assess the details of the decoherence process governing the dynamics of qubits interacting with spin environments. Analytical results and coherent state numerical techniques (similar to those pioneered in quantum optics by R. Glauber) have also been developed and applied. Most recently, specific strategies for quantum control have been investigated for realistic systems in order to extend the coherence times for spin-based quantum computing implementations. Many of the investigations were motivated by recent laboratory results and were studied and driven via interactions with experimental groups supported by the QC program. 14 publications were produced, 18 invited talks given, and 4 postdocs were trained.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

1. W. Zhang, V. V. Dobrovitski, B. N. Harmon, L. F. Santos, and L. Viola, "Suppression of electron spin decoherence in a quantum dot" J. Mod. Opt. (2007, in press)

2. W. Zhang, N. Konstantinidis, K. A. Al-Hassanieh, and V. V. Dobrovitski, J. Phys.: Cond. Matter 19, 083202 (2007).

3. W. Zhang, V. V. Dobrovitski, B. N. Harmon, L. F. Santos, and L. Viola, Phys. Rev. B 75, 201302 (2007).

4. K. A. Al-Hassanieh, V. V. Dobrovitski, E. Dagotto, and B. N. Harmon, Phys. Rev. Lett. 97, 037204 (2006).

5. W. Zhang, K. A. Al-Hassanieh, V. V. Dobrovitski, E. Dagotto, B. N. Harmon, Phys. Rev. B 74, 205313 (2006).

6. V. V. Dobrovitski, J. M. Taylor, and M. D. Lukin, Phys. Rev. B 73, 245318 (2006)

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8. J. Lages, V. V. Dobrovitski, M. I. Katsnelson, H. A. De Raedt, and B. N. Harmon, Phys. Rev. E 72, 026225 (2005).

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(c) Presentations

1. W. Zhang, V. V. Dobrovitski, N. Konstantinidis, L. F. Santos, L. Viola, B. N. Harmon, "Coherence control via dynamical decoupling of an electron spin in a quantum dot", APS March Meeting, March 2007, Denver, CO

2. V. Dobrovitski, "Modeling of decoherence in quantum spin systems", 2007 Aspen Winter Conference on Condensed Matter Physics, January 2007, Aspen, CO

3. V. Dobrovitski, W. Zhang, B. N. Harmon, L. Viola, L. F. Santos, "Dynamical decoupling protocols for the electron spins in quantum dots", 37th Conference on The Physics of Quantum Electronics, January 2007, Snowbird, UT

4. W. Zhang, V. Dobrovitski, B. N. Harmon, "Dynamical control of two-level system's decay into continuum" 37th Conference on The Physics of Quantum Electronics, January 2007, Snowbird, UT

5. V. Dobrovitski, "Modeling Decoherence in Quantum Spin Systems", APS March Meeting, March 2006, Baltimore, MD

6. B. N. Harmon, "First Principles Calculations and Spin Models", APS March Meeting, March 2006, Baltimore, MD

7. W. Zhang, K. A. Al-Hassanieh, V. V. Dobrovitski, E. Dagotto, and B. N. Harmon, "Spin decoherence of an electron in quantum dot with external magnetic field through hyperfine coupling to nuclear spin bath", APS March meeting, March 2006, Baltimore, MD

8. V. V. Dobrovitski, B. N. Harmon, K. A. Al-Hassanieh, and E. Dagotto, "Numerical modeling of the central spin problem using the spin coherent states P-representation", Conference on Quantum Computations and Many-Body Systems, February 2006, Key West, FL

9. B. N. Harmon, "Quantum Decoherence in Simple Spin Systems", Midwest Solid State Physics Conference, October 2005, Columbia, MO

10. K. A. Al-Hassanieh, V. V. Dobrovitski, E. Dagotto, B. N. Harmon, "Relaxation of the Electron Spin in a Quantum Dot due to the Interaction with the Nuclear Spin Bath", APS March Meeting, March 2005, Los Angeles, CA

11. V. V. Dobrovitski, J. M. Taylor, M. D. Lukin, "Fidelity of the long-lived memory for mesoscopic quantum bits", APS March Meeting, March 2005, Los Angeles, CA

12. J. Lages and V. V. Dobrovitski, "Decoherence of few-spin systems by a chaotic spin bath", APS March meeting, March 2004, Montreal, Canada

13. V. V. Dobrovitski and B. N. Harmon, "Modeling Rabi oscillations in a Josephson junction qubit with a defect", APS March meeting, March 2004, Montreal, Canada

14. B. N. Harmon, "From Molecular Nanomagnetis to Interacting Quantum Qubits", February 2004, Chemical Physics Workshop,

University of Tennessee, Knoxville, TN

15. V. V. Dobrovitski, H. A. De Raedt, M. I. Katsnelson, and B. N. Harmon, "Numerical simulations of decoherence in many-spin systems", February 2004, Gordon Research Conference 2004, Ventura, CA.

16. V. V. Dobrovitski and B. N. Harmon, "Decoherence of many-spin systems: numerical and analytical studies", Workshop on Theory in Quantum Computations, July 2003, Harpers Ferry, WV

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(d) Manuscripts

1. W. Zhang, V. V. Dobrovitski, B. N. Harmon, L. F. Santos, and L. Viola, "Extending coherence time for an electron spin in a quantum dot via dynamical decoupling method", Phys. Rev. B (submitted)

2. Ren-Shou Huang, B. N. Harmon, and V. V. Dobrovitski, "Single qubit Rabi oscillations decohered by many two-level systems", manuscript cond-mat/0504449 on eprint server aps.arXiv.org.

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Number of Inventions:

Graduate Students

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Jose Lages	0.22
Ren-Shou Huang	0.27
Nikolaos Konstantinidis	0.31
Wenxian Zhang	0.34
FTE Equivalent:	**1.14**
Total Number:	**4**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Bruce N. Harmon	0.04	No
FTE Equivalent:	**0.04**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

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Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME
Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED	
Viatcheslav V. Dobrovitski	0.40	No
FTE Equivalent:	**0.40**	
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Foreword

This project has developed and used advanced high-precision numerical techniques to accurately assess the details of the decoherence process governing the dynamics of qubits interacting with spin environments. Analytical results and coherent state numerical techniques (similar to those pioneered in quantum optics by R. Glauber) have also been developed and applied. Most recently, specific strategies for quantum control have been investigated for realistic systems in order to extend the coherence times for spin-based quantum computing implementations. Many of the investigations were motivated by recent laboratory results and were studied and driven via interactions with experimental groups supported by the QC program. 14 publications were produced, 18 invited talks given, and 4 postdocs were trained.

Statement of the problem. Decoherence in solid-state spin-based qubit systems

The promise of quantum computers to solve classically non-computable problems [1] has generated great excitement and much research activity in different areas of physics, mathematics and engineering. Various physical systems have been proposed for implementation of quantum bits (qubits) in quantum information processing devices: trapped ions, atoms in QED cavities, magnetic molecules, etc. Among many candidates, spin-based solid-state systems, such as quantum dots [2] or spin centers in host crystals (phosphorus donors in silicon [3], NV centers in diamonds [4]), constitute attractive candidates for qubits: these systems are well scalable, can be fabricated and operated by the methods of modern microelectronics, and advanced spin-resonance techniques are well-suited for efficient quantum state manipulation. Thus, it is not surprising that a large number of leading research groups, both theoretical and experimental, focus their studies on developing and investigating solid-state spin-based qubits.

Along with advantages, solid-state systems present serious challenges. The most important one is the destructive influence of the environment, causing decoherence. For example, an electron spin 1/2 in a GaAs quantum dot, representing a quantum bit, always interacts with the nuclear spins of Ga and As (via the contact hyperfine coupling). The nuclear spins create a random time-varying magnetic field acting on the electron, which quickly (within 10 ns) destroys the subtle phase coherence between the electron spin states “up” and “down”, so that the quantum properties of the electron spin are lost [5]. In order to avoid such a rapid deterioration of qubit coherence, is it crucial that we understand the detailed dynamics of decoherence and find efficient ways of mitigating it.

Studying decoherence in solid-state spin-based qubit systems was the focus of our project. Since decoherence is a complex many-body non-equilibrium process, and its description by purely analytical means is rarely possible, our main tool was direct and highly accurate numerical solution of the time-dependent Schrodinger equation for the whole system (qubits plus their environment). This is a very difficult but extremely reliable approach, involving no approximations about the system or environment.

Working in conjunction with experimental and other theoretical groups involved in the QC program, we have investigated decoherence for a number of experimental systems, including: (i) electron spins decohered by the bath of nuclear spins in quantum dots and in magnetic molecules, (ii) decoherence of electronic donor spins and nuclear spins in silicon and in calcium fluoride, and (iii) Rabi oscillations decay in Josephson junctions. We have also answered several fundamental questions in the theory of decoherence, clarifying the effect of the internal dynamics of the bath and the system on the decoherence dynamics. Moreover, we have studied in detail different ways of mitigating decoherence, by using a quantum memory protocol, and by using quantum control for dynamical decoupling of the qubits from their environments. As a result, we have developed a detailed theoretical picture for many important aspects of decoherence in relevant spin-based qubit systems.

Description of main results and their relevance to QC program

During the period of the project, we have worked in close contact with experimental and theoretical groups within the QC program and outside. We used state-of-the-art numerical simulations [6-8] and realistic models for decohering environments, going beyond standard approximations which often are too restrictive. We performed research along the lines described in the initial proposal and later presented at the QC Program Reviews. Along with studying specific experimental systems, we also investigated fundamental problems in the theory of decoherence. Moreover, we developed a novel approach, based on diagonal representation of the density matrix, which allows modeling of decoherence in very large systems, with baths comprising thousands of spins. Our results have been described in 14 papers and manuscripts, including the topical review on modeling of decoherence in spin systems commissioned by the editors of Journal of Physics [7], and in 18 invited talks at conferences and research institutions internationally. Our main results, and their relevance for the QC program, are explained in detail below.

1. Quantum dots: decoherence dynamics and quantum control

Much of our effort was directed at studying electron spins in quantum dots decohered by the nuclear spin bath. This research has been motivated by impressive experimental progress in this area, in particular, by the experiments of C. Marcus's group (funded by QC program) on relaxation in quantum dots mediated by nuclear spins [5]. Decoherence by a bath of nuclear spins is dominant in typical experiments, at moderate magnetic fields and low temperatures. We investigated in detail the electron spin decoherence and Rabi oscillations for various fields and bath polarizations, for both short and long times [7-12]. We have demonstrated [7,8] that the decoherence of a single electron at long times has a very unusual, logarithmic form, $1/\ln t$, as shown in Fig. 1 (in these works, we have used a novel method for modeling decoherence by very large baths, based on diagonal representation of the density matrix, see Sec. 3 below). This work prompted J. Taylor from the experimental group of C. Marcus and M. Lukin (funded

by QC program) to look into the long-time decay of the electron spins in quantum dots. Unfortunately, due to technical problems, their conclusions were not certain: the experiments did not disprove this prediction, but also did not clearly confirm it (the problem was the long-time stability of the experimental setup: confirmation of logarithmic decay requires the complex apparatus to keep the same voltages for few days, which is difficult). Furthermore, using advanced numerical simulations, we analyzed the decoherence dynamics in the experimentally relevant situation of moderate and small fields and bath polarizations, which can not be studied with standard analytical methods. We identified several qualitatively different regimes of decoherence, and suggested possible experiments which can verify our predictions [9]. Moreover, studying the influence of the bath polarization on the electron spin decoherence, we found that experimentally relevant small-to-intermediate polarization (below 90%) does not extend coherence time, and therefore polarizing the nuclear bath (which has been suggested by some groups) is not a viable way for fighting decoherence.

In order to slow down the coherence decay, various approaches can be used. A simple approach is to modify the system's Hamiltonian, in order to reduce the coupling to the bath, e.g. by applying a strong field (essentially, implementing the Rabi oscillations experiment with sufficiently strong driving field). We have studied this situation, and have predicted that in case of a sufficiently strong driving field, Rabi oscillations demonstrate an unusual, slow, power-law decay ($A \sim t^{-1/2}$, where A is the oscillation amplitude and t is time) [10] instead of fast Gaussian damping (which takes place without strong driving). This prediction has recently been clearly confirmed in experiments [13]. We also proposed a similar scheme for two quantum dots (or any even number of dots) [11,12], where the role of strong driving is assumed by strong exchange coupling between electron spins. While in general the coherence time decreases exponentially with the number of qubits, we have shown that, in some regimes, decoherence of several coupled qubits can be slower than decoherence of a single qubit. These findings are relevant for future experiments on coupled quantum dots.

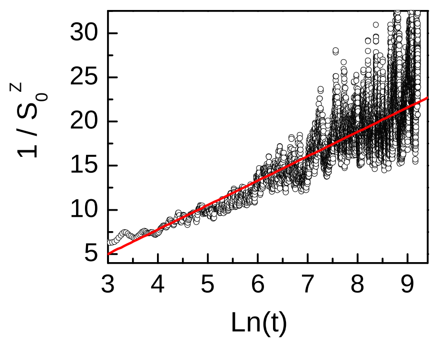

Fig. 1. Decay of z-component of the electron spin S_0 due to decoherence by a bath of nuclear spins. Graph clearly shows linear dependence of $1/S_0^z$ on ln(t) over about 3 decades in time.

Decoherence can be mitigated more efficiently by more advanced (although more complex) methods of quantum control, using dynamical decoupling of the system from its environment. This decoupling can be achieved by applying a specially designed protocol: a sequence of pulses affecting the system in such a way that its coupling to the bath spins is significantly reduced. This approach has been

actively studied by many groups (including groups of D. Lidar, L. Sham and S. Das Sarma, funded by QC program) [14,15], but their previous studies have been focused on the case of strong magnetic field applied to the dots, where the relaxation of the electron spin can be neglected, and a large part of the work can be performed analytically. We focused on the more complex, but more experimentally relevant case of low-to-moderate magnetic fields, where both relaxation and dephasing of the spin are present. By using advanced numerical methods, we have extensively studied a series of different decoupling protocols, deterministic and randomized [16-18]. We found that some advanced pulse sequences perform extremely well for electron spins in quantum dots, protecting coherence with very high precision and reducing the decoherence rate by a factor of several thousands. Moreover, our numerical approach has allowed studying the performance of the dynamical decoupling protocols at large times and large inter-pulse delays, far beyond the region of applicability of standard analytical approaches. Earlier analytical estimates [14] severely restricted the region of applicability of the dynamical decoupling, requiring the inter-pulse delay to be in the picosecond range. We found [16-18] that, contrary to these expectations, the inter-pulse delay can be made much larger, in the nanosecond range, without noticeable deterioration of performance of decoupling. These results clearly demonstrate that the dynamical decoupling is a viable way for fighting decoherence in quantum dots even at low-to-moderate magnetic fields.

Finally, instead of fighting the nuclear spin bath, one can rather harness it for quantum information storage, as proposed by the group of M. Lukin and C. Marcus [19] (funded by QC program). In collaboration with M. Lukin's group, we studied the quantum memory in detail, taking into account unavoidable experimental errors (incomplete polarization of the bath and inhomogeneous coupling to the nuclear spins). We found that fidelity of the memory protocol is good (~80%) for reasonably large bath polarizations (~80 %), and with further experimental progress, the quantum memory may be practical.

2. Modeling of nuclear magnetic resonance systems

Decoherence in many-qubit systems with complex dynamics.

Nuclear magnetic resonance (NMR) experiments provide an excellent testground for many crucial concepts of quantum information processing: from first proof-of-principles demonstration of quantum computation [20] to the studies of quantum control and dynamical decoupling [21,22], and fundamental questions of decoherence theory. We have devoted considerable effort to theoretical understanding and numerical modeling of these issues.

In close interaction with the experimental groups of S. Barrett and of S. Lyon and A. Tyryshkin (both funded by the QC program), we have studied the experiments on unusual spin echo in ^{29}Si NMR found by the group of S. Barrett [21]. These experiments have shown that the system of many coupled spins 1/2 (i.e., many coupled qubits) subjected to a train of dynamical decoupling pulses exhibits an unusual long tail of spin echoes and an unexpected large difference between the even and odd echo

amplitudes. Since dynamical decoupling (see also Sec. 1 above) is an important tool for fighting decoherence, possible artifacts of this technique should be understood in detail. We have modeled these experiments, and excluded several possibilities (e.g., that the observed effect is due to spin locking at low pulse fields). We have offered a possible explanation [7], showing that unusual echoes appear in generic dipolar-coupled spin systems at low control fields as a result of non-ideal control pulses. Our work prompted the group of S. Lyon/A. Tyryshkin and of S. Barrett to perform a series of follow-up experiments [22] on various systems. While the final explanation is not given yet, but both theory and experiments demonstrate that the observed behavior is relevant for a wide range of many-qubit systems with complex internal dynamics (see e.g. magnetic molecules in Sec. 4 below).

This work brought up an interesting and important issue of the role of complex internal dynamics of the system or bath in the process of decoherence. Many standard theoretical approaches to decoherence describe the influence of the bath in a simplified manner, using only a few parameters (the strength of system-bath coupling, characteristic energies/times of the bath, etc.). However, it has been noted [23] (the group of W. Zurek was funded by QC program) that such a treatment may sometimes be misleading, and the details of the bath dynamics may be crucial. In particular, there is a qualitative difference in decoherence by a bath possessing very complex (chaotic) internal dynamics and the same bath with regular (integrable) dynamics. The onset of quantum chaos in spin baths is caused by coupling between the bath spins, and may happen already at very small coupling magnitudes, thus making the issue important for a wide range of real systems/baths (including e.g. quantum dots or Si:P systems, actively studied by several groups in the QC program). Previous works [23], however, treated the joint system-bath dynamics in a simplified way, leading to a number of controversies and debates. By performing approximation-free numerical simulations with sufficiently complex systems and baths [24,25], we have shown that the intuitive arguments, while formally incorrect, still give a qualitatively correct answer to the problem: indeed, the onset of quantum chaos leads to significantly faster and stronger decoherence, in spite of the fact that the system-bath coupling strength and the characteristic energies of the bath remain roughly the same for both chaotic and regular regimes.

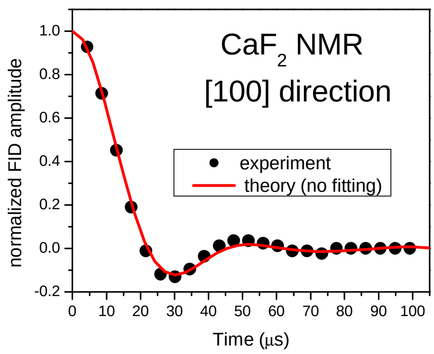

Fig. 2. Modeling of free induction decay in CaF_2: comparison between experiment and numerical simulations. The simulations reproduce correctly fine details of the experimental curves, such as small oscillations at longer times.

The next step in this direction has become possible during the final year of the project, when we developed a new method of decoherence simulations, which allowed modeling of realistically large

systems (thousands of quantum spins, see Sec. 3 below) with complex dynamics. In particular, we have modeled [7] the free induction decay of NMR signal in CaF_2 crystals, with 27,000 quantum spins 1/2, all coupled together by dipolar interactions. Our simulations reproduced even the fine details of dynamics of such a complex system without a single adjustable parameter (see Fig. 2). Although this project is not funded by QC program anymore, we are still pursuing this interesting direction, studying the details of decoherence in different large complex systems.

3. Development of methods for numerical modeling of decoherence.

A noticeable part of our studies has become possible due to progress in methods for numerical modeling of decoherence. In most simulations, we used a direct approach: we represented the wavefunction for the total system (the central system plus the bath spins) as a many-dimensional vector in a Hilbert space (with dimensionality 2^N where N is the total number of spins in the system and in bath), and modeled evolution of this vector by directly solving the Schrodinger equation. Since the number of spins (20-30) in our simulations was rather large, the required memory and time resources were significant (e.g., 30 spin simulations require 48 GB of RAM). Special numerical and programming techniques were used to make the simulations possible [6,7]. Special software was also developed for parallel computations. While very demanding, this approach has important advantages: it is exact, it is applicable to any system (if the system is sufficiently small), and it does not involve any approximations.

On the other hand, in some situations, in order to obtain reliable results, we need to model thousands of spins (e.g., in order to study the long-time decoherence of the electron spins in quantum dots, Sec. 1, or model the solid-state NMR experiments, Sec. 2). Fortunately, within the present project, we managed to develop an approach which can handle such simulations [7,8]. This approach is based on the diagonal representation (so-called P-representation) of the many-spin density matrix in the basis of spin coherent states, and allows reformulation of the many-spin dynamics in terms of classical Monte-Carlo sampling in the space of classical trajectories. In spite of being approximate, this approach provides excellent accuracy, as confirmed by comparison with experiments and with our independent exact simulations, and is applicable to various systems with different Hamiltonians.

4. Other systems

Among other systems studied within the present project, we investigated decoherence of electron spin in magnetic molecules by a bath of nuclear spins [26]. The possibility of using magnetic molecules as qubits has been studied within the QC program by the group of D. Allara / G. Doolen / G. Berman, but our work is focused on different aspects of spin decoherence in magnetic molecules. The goal of our work was to understand how the interactions between the nuclear spins in magnetic molecules affect the decoherence process (see also Sec. 2 above). We studied decoherence in two important situations: during the spin-flip of the electronic spin in a static external field (which is similar to the single-qubit NOT operation) and

during the spin-flip in a linearly varying external field, at the level crossing (which is used for readout in many schemes for quantum computing, e.g. in Si:P proposal [3]). We have shown that the internal dynamics of the bath strongly affects the process of decoherence, and that the standard approximate model of the random fluctuating magnetic field can not describe the decoherence process adequately.

We also studied the visibility and the decay of Rabi oscillations in Josephson junction qubits. An important experimental problem is why the amplitude of the Rabi oscillations is small (rarely exceeding 40-50 %) although the decay time may be quite long. The decoherence of superconducting qubits is not completely understood yet, but the experimental evidence [27] from J. Martinis's group (funded by QC program) show that the bath of two-level fluctuators (which is equivalent to a bath of spins 1/2) is an important source of decoherence. Theoretical investigation of the Rabi oscillations damped by the bath of two-level fluctuators has been performed by several groups within the QC program, and is directly relevant to numerous experiments on superconducting qubits funded by the QC program. We have shown [28] that the amplitude and the decay time for Rabi oscillations may be governed by different groups of fluctuators. The fluctuators with frequencies different from the frequency of the qubit strongly affect the visibility but have small effect on the oscillations decay time, while the fluctuators with frequencies close to the qubit frequency govern the oscillations decay.

Summary

Withing the present project, we used numerical simulations, as well as a number of analytical tools, to study decoherence in various spin systems, such as quantum dots, different NMR systems, magnetic molecules, etc. We have also investigated important fundamental problems of decoherence theory. Working in close contact with experimental and theoretical groups within and outside the QC program, we have studied the dynamics of decoherence in free systems, and have investigated different ways of fighting decoherence, by modifying the system's Hamiltonian and by using the dynamical decoupling techniques based on quantum control methods. As a result, we have provided a detailed theoretical description for many important aspects of decoherence in systems relevant for quantum information processing.

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